

Field dependent equilibrium energetic distribution of localized charge carriers in disordered semiconductors at low temperatures.

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The hopping transport of charge carries in 3-dimensional disordered semiconductors is analyzed in this work. It is assumed that the density of localized states is a decreasing function of energy and contribution of thermoactivated jumps into the transport is negligible. The possibility of equilibrium energetic distribution for this case is shown. This distribution is characterized by field-dependent effective temperature.

Processes of carrier transport in amorphous semiconductors with conduction via delocalized states have been successfully described in terms of the multiple-trapping model [1-3]. This model implies that two carrier fractions exist in the material, occupying at any given instant of time delocalized and localized states. However, in the materials with all carriers in localized states, e.g., in most polymers, charge transport is due to carrier hopping. Many interesting and important features of the hopping transport in disordered semiconductors have been observed experimentally in fairly high electric fields [4-6]. It has been shown both analytically [7-10] and by Monte Carlo simulations [11, 12] that the energy distribution of localized carriers and the carrier mobility in a disordered semiconductor can be described both by the ordinary temperature T and by some effective temperature $T_F(F)$ dependent on the magnitude of the applied external electric field F . Analytical calculations [7, 9] of this effective temperature yield

$$T_F = \frac{eF}{2\gamma k}, \quad (1)$$

while numerical simulation yields $T_F = 0.67 \cdot eF/\gamma k$ (see [11]) or $T_F = (0.69 \pm 0.03) \cdot eF/\gamma k$ (see [12]), where e is the elementary charge, $1/\gamma$ the localization radius, and k the Boltzmann constant. The equilibrium energy distribution of injected carriers in an amorphous semiconductor subjected to an external electric field at low temperatures, when the contribution of thermally activated hops to the transport process is negligible, has been found [9] for the 1D case, which, in fact, corresponds to high electric fields. In this paper, we demonstrate that the equilibrium energy distribution of localized carriers is also possible in the 3D case at low temperatures in an external electric field. We show that this distribution can be described by the Boltzmann exponential with an effective temperature given by (1).

As an equation describing the kinetics of the hopping

transport, we use the well-known balance equation

$$\frac{\partial f_i}{\partial t} = \sum_{j \neq i} \nu_{ji} f_j - f_i \sum_{j \neq i} \nu_{ij}, \quad (2)$$

written for the case of low occupancy of localized states, $f_i \ll 1$. Here, t is the time, f_i the mean occupation number of the i -th state and ν_{ij} the probability of transition from the state i to the state j . Let us assume that in the quasiequilibrium transport regime, when the density of states is time-independent, a great number of carriers can avoid unlikely jumps that take a very long time $t_R \gg \hbar/\Delta E$, i.e., jumps that do not contribute significantly to the transport process [13]. Here, \hbar is Planck's constant and ΔE the characteristic energy change in carrier transition from one localized state to another. This assumption makes it possible to take advantage of the concept of the distribution function $f(\mathbf{r}, E, t)$ averaged over continuous variables: energy E ("deeper" states have higher energies E) and radius vector \mathbf{r} . Let us use the Miller-Abrahams expression for the transition rate

$$\nu(|\Delta \mathbf{r}|, E) = \nu_0 \exp \left(-2\gamma |\Delta \mathbf{r}| - H(\mathcal{E}) \frac{\mathcal{E}}{kT} \right), \quad (3)$$

where $\mathcal{E} \equiv E - e\mathbf{F}\Delta \mathbf{r} - E'$, $H(\mathcal{E})$ is the Heaviside function, ν_0 the attempt-to-jump frequency, and $\Delta \mathbf{r} = \mathbf{r} - \mathbf{r}'$. Then, we use equation derive the following kinetic equation for the distribution function f ,

$$\begin{aligned} \frac{\partial f(\mathbf{r}, E, t)}{\partial t} = & \nu_0 \int d\mathbf{r}' \exp(-2\gamma |\Delta \mathbf{r}|) g(E) \times \\ & \left[\int_{E-e\mathbf{F}\Delta \mathbf{r}}^{\infty} dE' \exp\left(\frac{E - e\mathbf{F}\Delta \mathbf{r} - E'}{kT}\right) f(\mathbf{r}', E', t) \right. \\ & \left. + \int_{-\infty}^{E-e\mathbf{F}\Delta \mathbf{r}} dE' f(\mathbf{r}, E', t) \right] - \\ & \nu_0 \int d\mathbf{r}' \exp(-2\gamma |\Delta \mathbf{r}|) f(\mathbf{r}, E, t) \times \\ & \left[\int_{-\infty}^{E-e\mathbf{F}\Delta \mathbf{r}} dE' \exp\left(\frac{-[E - e\mathbf{F}\Delta \mathbf{r} - E']}{kT}\right) g(E') \right] \end{aligned}$$

$$+ \int_{E-e\mathbf{F}\Delta\mathbf{r}}^{\infty} dE' g(E') \Big], \quad (4)$$

by the condition

$$\int d\mathbf{r} \int_{-\infty}^{\infty} f(\mathbf{r}, E, t) dE = 1, \quad (5)$$

where $g(E)$ is the energy distribution of localized states (DOS) normalized by the condition

$$\int_{-\infty}^{\infty} g(E) dE = 1. \quad (6)$$

The zero energy $E = 0$ corresponds to the maximum of the function $g(E)$. Equation (4) is written on the assumption that the position and energy of localized states are uncorrelated, which corresponds to the case of completely disordered materials.

At low temperatures, when the contribution of thermally activated hops can be neglected subject to the condition of hypothetical equilibrium, kinetic equation (4) for the equilibrium distribution function averaged over the space coordinates

$$f_{eq}(E) = \int f(\mathbf{r}, E, \infty) d\mathbf{r} \quad (7)$$

takes the form

$$0 = \nu_0 \int d\mathbf{r}' \exp(-2\gamma|\Delta\mathbf{r}|) \int_{-\infty}^{E-e\mathbf{F}\Delta\mathbf{r}} dE' f_{eq}(E') g(E) - \nu_0 \int d\mathbf{r}' \exp(-2\gamma|\Delta\mathbf{r}|) \int_{E-e\mathbf{F}\Delta\mathbf{r}}^{\infty} dE' g(E') f_{eq}(E). \quad (8)$$

We use equation (8) and formulas (5) and (6) to derive the following integral equation:

$$f_{eq}(\varepsilon) = g(\varepsilon) \frac{A(\varepsilon, \varepsilon') f_{eq}(\varepsilon')}{4 - A(\varepsilon, \varepsilon') g(\varepsilon')}. \quad (9)$$

Here, we introduced the integrated operator

$$A(\varepsilon, \varepsilon') = \int_{-\infty}^{\infty} d\varepsilon' \left[4H(\varepsilon - \varepsilon') - \text{sgn}(\varepsilon - \varepsilon') (2 + |\varepsilon - \varepsilon'|) e^{-|\varepsilon - \varepsilon'|} \right], \quad (10)$$

and the dimensionless variables $\varepsilon = E/kT_F$ and $\varepsilon' = E'/kT_F$, where T_F is the effective temperature defined by (1). The appearance of this effective temperature is associated with the fact that, during transport, the electric field transfers carriers into states with a higher energy, similarly to the thermodynamic effects described by the ordinary temperature T .

This equation can be solved by the iteration method; as the first approximation, we use the density of localized states

$$f_{eq}^{(0)}(E) = g(E). \quad (11)$$

Substituting (11) into (9), we obtain

$$A(\varepsilon, \varepsilon') g(\varepsilon') \sim \begin{cases} 4 - \varepsilon e^{-\varepsilon}, & E \gg E_0 + E_m(T_F); \\ -\varepsilon e^{\varepsilon}, & E \ll -E_0 - E_m(T_F). \end{cases} \quad (12)$$

Here, the quantity $E_m(T_F)$ depends on the particular form of the DOS function. In particular, in the case of a Gaussian distribution

$$g(E) = g_0 \exp(-[E/E_0]^2),$$

we have $E_m(T_F) = E_0^2/2T_F$, while in the case of an exponential distribution

$$g(E) = g_0 \exp(-|E/E_0|)$$

we obtain $E_m(T_F) = E_0^2/(T_F - E_0)$.

Hence,

$$f_{eq}^{(1)}(E) \sim |E|^{-\text{sgn}(E)} g(E) \exp\left(\frac{E}{kT_F}\right),$$

$$|E| \gg E_0 + E_m(T_F). \quad (13)$$

Thus, to a first approximation, the equilibrium energy distribution is described by the Boltzmann function. To calculate the distribution function $f_{eq}(E)$ more precisely, we substitute, in accordance with (13), the function $g(E) \exp(E/kT_F)$ into the right-hand side of equation (9). The resulting solution $f_{eq}^{(2)}(E)$ has the same asymptotic form as the function $f_{eq}^{(1)}(E)$, since the asymptotic form (12) of the function $A(\varepsilon, \varepsilon') g(\varepsilon')$ appearing in equation (9) is not changed. Thus, if the DOS function $g(E)$ is sufficiently "shallow", so that the equilibrium can be established,

$$E g(E) \exp\left(\frac{E}{kT_F}\right) \rightarrow 0, \quad |E| \rightarrow \infty, \quad (14)$$

then the asymptotic form of the occupancy of localized states $\varphi(E) = f(E)/g(E)$ is the exponential $\exp(E/kT_F)$. The quantity $E_m(T_F)$ appearing in equations (12) and (13) is the characteristic energy of the peak in the distribution function $f_{eq}(E)$.

Thus, we showed the following. First, in the 3D case, as also in the 1D one [9], the spatially uniform equilibrium energy distribution of localized charge carriers may occur even in the limiting case $T \rightarrow 0$, when the contribution from thermally activated hops to the kinetic equation (4) can be completely neglected. Second, this distribution can be approximated by the Boltzmann distribution function with the effective temperature (1) instead of the ordinary temperature. It should be noted

that this effective temperature coincides with previous analytical estimations [9, 10].

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